

BV-BRC Test Report

D10. Protein Structures Data Tab

Item to test	Protein Structures Data Tab
URL	https://www.bv-brc.org/view/Taxonomy/194#view_tab=features
Prerequisites	None
References	https://www.bv-brc.org/docs/quick_references/organisms_taxon/protein_structures.html
Tester(s)	Rebecca Wattam, Richard Scheuermann, Ron Kenyon
Test date	6-Jan-2022 and 4-Feb-22 (original – partial success), 9-May-2022 (follow-up-passed)
Test result	Passed

Overview

- Test the Protein Structures Tab with example bacterial and viral data.
- Verify structures exist.
- Test Structure action button.
- Test example structure operations.

Test Results

- Test results were verified by examination of returned data via inspection and filters.
- All operations performed as expected.
- Future enhancement:
 - Issue: Parse gene names and resolution from PDB metadata.
 - Resolution: Updated the data loader to populate gene names and resolution from PDB metadata.

Bacteria

Mycobacterium:

Check of existence: Sum of Methods equals total count

Taxon View

Bacteria » Actinobacteria » Actinomycetia » Corynebacteriales » Mycobacteriaceae » Mycobacterium (33401 Genomes)

Overview

Phylogeny

Taxonomy

Genomes

AMR Phenotypes

Sequences

Proteins

Protein Structures

Specialty Genes

Domains and Motifs

Epitopes

Pathway

Download

KEYWORDS

ADV Search

HIDE

Organism Name	Gene	Method	Institution
Mycobacterium tuberculosis H37Rv (3)	A7U43_17735 (1)	Electron microscopy (63)	(TBSGC) (1)
Archaeoglobus fulgidus (2)	BQ2027_MB1858 (1)	Solid-state nmr (1)	Accelerated Technologies Center for Gene to 3D Structure (/
Bacillus phage PBS2 (1)	BZL29_7639 (3)	Solution nmr (71)	Center for Structural Genomics of Infectious Diseases (CSG
Enterobacteria phage T4 (1)	CAB90_01754 (1)	X-ray diffraction (2927)	Integrated Center for Structure and Function Innovation (ISF
Escherichia coli (4)	CKJ66_17020 (1)		Israel Structural Proteomics Center (ISPC) (1)
Escherichia coli K-12 (1)	E5M05_02265 (1)		Midwest Center for Structural Genomics (MCSG) (3)
Homo sapiens (2)	E5M05_10720 (1)		Mycobacterium Tuberculosis Structural Proteomics Project (;
MYCOBACTERIUM AVIUM (1)	E5M05_13560 (4)		New York Consortium on Membrane Protein Structure (NYC
MYCOBACTERIUM BOVIS (1)	E5M05_13585 (1)		New York SGX Research Center for Structural Genomics (N'
MYCOBACTERIUM LEPRAE (3)	E5M05_14320 (1)		New York Structural Genomics Research Consortium (NYSG
MYCOBACTERIUM MARINUM (4)	E5M05_16060 (1)		Northeast Structural Genomics Consortium (NESG) (4)
MYCOBACTERIUM TUBERCULOSIS (322)	ERS007657_00996 (2)		Seattle Structural Genomics Center for Infectious Disease (S
MYCOBACTERIUM TUBERCULOSIS H37RV (11)	ERS007661_01687 (2)		Structural Proteomics in Europe (SPINE) (5)
Mycobacterium [tuberculosis] TKK-01-0051 (1)	I547_2743 (1)		Structures of Mtb Proteins Conferring Susceptibility to Knowi
Mycobacterium avium (33)	J113_05350 (1)		TB Structural Genomics Consortium (TBSGC) (322)
Mycobacterium avium (strain 104) (11)	J113_23825 (1)		

PDB ID	Title	Organism Name	BRC ID	UniProtKB Accession	Gene	Product	Method	Release Date
4W1U	Crystal structure of Rv3557c/KstR2, a transcr	Mycobacterium	fig 83332.642.peg.171	P9WMB9	kstR2	HTH-type transcriptional repressor KstR2	X-ray diffraction	2015-07-29T00:00:00
4WS5	Crystal structure of Mycobacterium tubercul	Mycobacterium	fig 83332.12.peg.332	P9WFO9	ung	Uracil-DNA glycosylase	X-ray diffraction	2015-07-15T00:00:00
4WS6	Crystal structure of Mycobacterium tubercul	Mycobacterium	fig 83332.12.peg.332	P9WFO9	ung	Uracil-DNA glycosylase	X-ray diffraction	2015-07-15T00:00:00
4WXT	X-ray crystal structure of thioredoxin from M	Mycobacterium	fig 1160712.3.peg.471	A0A067HW1	MAV3388_24025	Thioredoxin	X-ray diffraction	2014-11-26T00:00:00
4X58	Anthranilate phosphoribosyl transferase vari	Mycobacterium	fig 419947.9.peg.304	A5U4M0	trpD	Anthranilate phosphoribosyltransferase	X-ray diffraction	2015-11-25T00:00:00
4X59	Anthranilate phosphoribosyltransferase vari	Mycobacterium	fig 419947.9.peg.304	A5U4M0	trpD	Anthranilate phosphoribosyltransferase	X-ray diffraction	2015-11-25T00:00:00
4XGQ	Crystal structure of addition module from M	Mycobacterium	fig 83332.12.peg.696	P9WJ35,P9	vapB30,vapC30	Antitoxin VapB30,Ribonuclease VapC30	X-ray diffraction	2015-08-12T00:00:00
4XGR	Crystal structure of addition module from M	Mycobacterium	fig 83332.12.peg.696	P9WJ35,P9	vapB30,vapC30	Antitoxin VapB30,Ribonuclease VapC30	X-ray diffraction	2015-08-12T00:00:00
4XXP	Crystal Structure of an Uncharacterized Pro	Mycobacterium	patric_id	Q73ZE2	MAP_1661c	GH16 domain-containing protein	X-ray diffraction	2015-02-11T00:00:00
4XXX	Structure of PE-PPE domains of ESX-1 secr	Mycobacterium	fig 83332.12.peg.432	P9WJD9	espB	ESX-1 secretion-associated protein EspB	X-ray diffraction	2015-02-18T00:00:00
4Y12	Crystal structure of the S/T protein kinase P	Mycobacterium	fig 83332.12.peg.452	P9WI73	pknG	Serine/threonine-protein kinase PknG	X-ray diffraction	2015-05-20T00:00:00
4Y9X	Crystal structure of glucosyl-3-phosphoglyce	Mycobacterium	fig 83332.12.peg.135	P9WMW9	gpgS	Glucosyl-3-phosphoglycerate synthase	X-ray diffraction	2015-07-15T00:00:00
4YNR	DosS GAFA Domain Reduced CO Bound Cr	Mycobacterium	fig 419947.9.peg.388	P9WGK2	devS	Oxygen sensor histidine kinase response regulator Dev	X-ray diffraction	2016-02-24T00:00:00
4ZFQ	Structure of M. tuberculosis (3,3) L,D-Trans	Mycobacterium	fig 83331.22.peg.538	P9WKV2	MT0501	L,D-transpeptidase 5	X-ray diffraction	2015-09-02T00:00:00
4ZOK	Methylsulfonyl-containing inhibitor bound in	Mycobacterium	fig 419947.9.peg.304	A5U4M0	trpD	Anthranilate phosphoribosyltransferase	X-ray diffraction	2016-05-11T00:00:00
4ZTV	Non-anthranilate-like inhibitor (TAMU-A7) cc	Mycobacterium	fig 419947.9.peg.304	A5U4M0	trpD	Anthranilate phosphoribosyltransferase	X-ray diffraction	2016-05-25T00:00:00
5BO3	Bianthranilate-like inhibitor with 5 atom "line"	Mycobacterium	fig 419947.9.peg.304	A5U4M0	trpD	Anthranilate phosphoribosyltransferase	X-ray diffraction	2016-06-01T00:00:00
5BTC	Crystal structure of a topoisomerase II com	Mycobacterium	fig 83332.115.peg.5	P9WG47,P9	gyrA,gyrB	DNA gyrase subunit A,DNA gyrase subunit B	X-ray diffraction	2016-03-02T00:00:00
5BTF	Crystal structure of a topoisomerase II com	Mycobacterium	fig 419947.63.peg.6	P9WG45,P9	gyrB,gyrA	DNA gyrase subunit B,DNA gyrase subunit A	X-ray diffraction	2016-03-02T00:00:00
5BYT	PRPP complexed with a single Mg in the act	Mycobacterium	fig 419947.9.peg.304	P9WFX5	trpD	Anthranilate phosphoribosyltransferase	X-ray diffraction	2016-07-20T00:00:00
5CJN	Crystal structure of Mycobacterium tubercul	Mycobacterium	fig 83332.12.peg.204	P9WK17	glcB	Malate synthase G	X-ray diffraction	2016-08-10T00:00:00

1 - 200 of 3062 results

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1

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3

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16

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Structure display:

☐	PDB ID	Title	Organism Name	BRC ID	UniProtKB Accession	Gene	Product	Method	Release Date
☐	4W1U	Crystal structure of Rv3557c/KstR2, a trans	Mycobacterium	fig 83332.642.peg.17	P9WMB9	kstR2	HTH-type transcriptional repressor KstR2	X-ray diffraction	2015-07-29T
☐	4WS5	Crystal structure of Mycobacterium tubercul	Mycobacterium	fig 83332.12.peg.332	P9WFG9	ung	Uracil-DNA glycosylase	X-ray diffraction	2015-07-15T
☒	4WS6	Crystal structure of Mycobacterium tubercul	Mycobacterium	fig 83332.12.peg.332	P9WFG9	ung	Uracil-DNA glycosylase	X-ray diffraction	2015-07-15T
☐	4WXT	X-ray crystal structure of thioredoxin from M	Mycobacterium	fig 1160712.3.peg.47	A0A067HW	MAV3388_24025	Thioredoxin	X-ray diffraction	2014-11-26T
☐	4X58	Anthranilate phosphoribosyl transferase vari	Mycobacterium	fig 419947.9.peg.304	A5U4M0	trpD	Anthranilate phosphoribosyltransferase	X-ray diffraction	2015-11-25T
☐	4X59	Anthranilate phosphoribosyltransferase vari	Mycobacterium	fig 419947.9.peg.304	A5U4M0	trpD	Anthranilate phosphoribosyltransferase	X-ray diffraction	2015-11-25T

4WS6

PDB ID

4WS6

Title

Crystal structure of Mycobacterium tuberculosis uracil-DNA glycosylase in complex with 5-aminouracil, Form I

Organism Name

Mycobacterium tuberculosis

Taxon ID

83332

Genome

83332.12

ID

Feature ID

PATRIC:83332.12.NC_000962.CDS.3332071.3332754

BRC ID

fig|83332.12.peg.3321

UniProtKB

P9WFG9

Accession

Gene

ung

Ligands

Highlight Ligands

Sequence of 4WS6 | Cryst...

Chain 1: Uracil-DNA...

MSHHHHHHGASHTARPLSELVERGNAALFPAQVAMNQFLRAEIAAGRYLPAGENVLAFTFFPDRVRLVQOQPTTPPGHAGVLSFSAPOVRFWFRSLANIFDEYTAOLGYPLPSNGD
LTFNAQGRVLLLRVLTVRPNFASBRGKEAVTECAIRALAAHAPLVAILMGROASTLKFMLAAGNCVAIESPHFSPLSASRGFTGSRFFSRANELLVGMGAEPIDNRLP

Structure Tools

Structure

4WS6 | 2 structures

Nothing Focused

Measurements

+ Add

Superposition

Chains

Atoms

Components

4WS6 | 2 structures

Preset

+ Add

Polymer

No repr.

Ligand

No repr.

Water

No repr.

Ion

Ball & Stick

Virus

Influenza: H7 HA

Taxon View

Viruses » Negamaviricota » Insthovicetes » Articulavirales » Orthomyxoviridae » Alphainfluenzavirus » Influenza A virus (810384 Genomes)

Overview

Taxonomy

Strains

Genomes

Proteins

Protein Structures

Domains and Motifs

Epitopes

Experiments

Surveillance

Serology

DOWNLOAD

"H7"

KEYWORDS ✕

ADV Search

HA

GENE ✕

Organism Name

Gene

Method

Homo sapiens (10)

HA (52)

Electron microscopy (2)

INFLUENZA VIRUS (A/TURKEY/ITALY/214845/2002 (H7N9)) (1)

NA (11)

X-ray diffraction (50)

INFLUENZA VIRUS A/ANHUI/1/2013 (H7N9) (6)

NS1 (1)

Influenza A virus (38)

PA (2)

Influenza A virus (A/Anhui/1-BALF_RG45/2013(H7N9)) (1)

PB1 (1)

Influenza A virus (A/Netherlands/219/2003(H7N7)) (3)

PB2 (1)

Influenza A virus (A/New York/107/2003(H7N2)) (1)

ns1 (4)

☐	PDB ID	Title	Organism Name	BRC ID	UniProtKB Accession	Gene	Product
☐	6WXL	Cryo-EM structure of the VRC315 clinical trial, vaccine-	Influenza A virus (/	fig 1395980.6.CDS.1	A0A067Y6L0,A	HA	Hemagglutinin
☐	6UIG	Crystal structure of human monoclonal antibody H7.20	Influenza A virus,H	fig 1481988.3.CDS.1	A0A4Y5QYN9	HA	Hemagglutinin
☐	6N5A	Crystal structure of an equine H7 hemagglutinin from A	Influenza A virus	fig 387227.6.peg.1	A0A348FV55,A	HA	Hemagglutinin
☐	6MLM	H7 HA0 in complex with Fv from H7.5 IgG	Influenza A virus (/	fig 519082.5.CDS.1	B2LVD7,B2LVD	HA	Hemagglutinin
☐	6II9	Crystal structure of H7 hemagglutinin from A/Anhui/1/2	Influenza A virus,H	fig 1332244.17.CDS.1	A0A0K1LUI9,A	HA	Hemagglutinin
☐	6II8	Crystal structure of H7 hemagglutinin from A/Anhui/1/2	Influenza A virus,H	fig 1663875.3.CDS.1	A0A024CX39,A	HA	Hemagglutinin
☐	6II4	Crystal structure of H7 hemagglutinin from A/Anhui/1/2	Influenza A virus,H	fig 1332244.17.CDS.1	A0A0K1LUI9,A	HA	Hemagglutinin
☐	6IDZ	Crystal structure of H7 hemagglutinin mutant H7-SVTQ	Influenza A virus	fig 1481988.3.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
☐	6IDD	Crystal structure of H7 hemagglutinin mutant SH1-AVP	Influenza A virus (/	fig 1332244.17.CDS.1	A0A088BEK2	HA	Hemagglutinin
☐	6IDB	Crystal structure of H7 hemagglutinin mutant H7-SVTQ	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
☐	6IDA	Crystal structure of H7 hemagglutinin mutant H7-SVTQ	Influenza A virus	fig 1481988.3.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
☐	6ID9	Crystal structure of H7 hemagglutinin mutant H7-SGTL	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
☐	6ID8	Crystal structure of H7 hemagglutinin mutant H7-SVTL	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
☐	6ID5	Crystal structure of H7 hemagglutinin mutant H7-SVPL	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
☐	6ID3	Crystal structure of H7 hemagglutinin mutant H7-SGPL	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
☐	6ID2	Crystal structure of H7 hemagglutinin mutant H7-AVTL	Influenza A virus	fig 1481988.3.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
☐	6ICY	Crystal structure of H7 hemagglutinin mutant H7-AGTL	Influenza A virus	fig 1481988.3.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
☐	6ICX	Crystal structure of H7 hemagglutinin mutant AH-AGPL	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
☐	6ICW	Crystal structure of H7 hemagglutinin mutant AH-SGTC	Influenza A virus	fig 1481988.3.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
☐	6FYU	Structure of H7(A/Shanghai/2/2013) Influenza Hemagg	Influenza A virus,L	fig 1332244.17.CDS.1	A0A4Y5QYN9	HA	Hemagglutinin
☐	6D8B	The crystal structure of hemagglutinin from A/Hong Kor	Influenza A virus	fig 11320.72129.CDS.1	A0A218MY65,A	HA	Hemagglutinin
☐	6D7U	The crystal structure of hemagglutinin from A/Guangdo	Influenza A virus	fig 11320.72161.CDS.1	A0A1S6R2B6,A	HA	Hemagglutinin
☐	6D7C	The crystal structure of hemagglutinin from A/Hong Kor	Influenza A virus	fig 1593637.6.CDS.1	S4V1Z7,A0A0C	HA	Hemagglutinin
☐	5VJM	Crystal structure of H7 hemagglutinin mutant (V186K, f	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
☐	5VJL	Crystal structure of H7 hemagglutinin mutant (V186K, f	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
☐	5VJK	Crystal structure of H7 hemagglutinin mutant (V186K, f	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin
☐	5VAG	Crystal structure of H7-specific antibody m826 in comp	Influenza A virus,H	fig 1332244.17.CDS.1	R4NN21	HA	Hemagglutinin
☐	5V2A	Crystal structure of Fab H7.167 in complex with influen	Influenza A virus (/	fig 1560294.3.CDS.1	A0A0R5TXT5,A	HA	Hemagglutinin
☐	5T6S	Crystal structure of the A/Shanghai/2/2013 (H7N9) influ	Influenza A virus	fig 1332244.17.CDS.1	R4NN21,R4NN	HA	Hemagglutinin

1 - 52 of 52 results

Structure:

6N5A

PDB ID

6N5A

Title

Crystal structure of an equine H7 hemagglutinin from A/equine/NY49/73 (H7N7)

Organism Name

Influenza A virus

Taxon ID

387227

Genome ID

387227.6

Feature ID

PATRIC.387227.6.LC414434.CDS.8.1720

BRC ID

fig|387227.6.peg.1

UniProtKB

A0A348FV55, A0A348FV55

Accession

Ligands

☐ Highlight Ligands

Sequence of 6N5A | Crysta... Chain 1: HEMAGGL... A ASM_1

ADPGDKICIGHAVSNGTKVDLTLEKGIENVNATETVEQNIIPKICSGKQTIDLGQCQLLGTITGPPQCDQFLEFSANLIERREGDDICYP

GKFDNEETLRKILRKSOGIKKENMGFTYTVQVITNGETISACRRSRSSSYAEMKWLISNTQWCVFPQMTKSYKNTKREPALLIWIHSGSTAEQ

TRLYGSGNKLITVWSSKYQQSFAPSPGPRPQINGQSGRIDFYWLMLDPNDTVTFSFNGAFIAPDRASFLRGKSLGQSDAQLDNNCEGECYHI



16:26:44 Updated Carbohydrate in 1ms.

16:26:44 Updated Ball & Stick in 2ms.

16:26:44 Updated Ball & Stick in 3ms.

Structure Tools

Structure

6N5A | 2 structures

Nothing Focused

Measurements

+ Add

Superposition

Chains Atoms

Components 6N5A | 2 structures

Preset + Add

Polymer

No repr.

Ligand

No repr.

Water

No repr.

Carbohydrate

2 reprs

Ion

Ball & Stick

Highlight ligands:

